

MONOTONICITY AND CONCAVITY PROPERTIES OF THE SPECTRAL SHIFT FUNCTION

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Dedicated with great pleasure to Sergio Albeverio on the occasion of his 60th birthday

ABSTRACT. Let H_0 and $V(s)$ be self-adjoint, V, V' continuously differentiable in trace norm with $V''(s) \geq 0$ for $s \in (s_1, s_2)$, and denote by $\{E_{H(s)}(\lambda)\}_{\lambda \in \mathbb{R}}$ the family of spectral projections of $H(s) = H_0 + V(s)$. Then we prove for given $\mu \in \mathbb{R}$, that $s \mapsto \text{tr}(V'(s)E_{H(s)}((-\infty, \mu)))$ is a nonincreasing function with respect to s , extending a result of Birman and Solomyak. Moreover, denoting by $\zeta(\mu, s) = \int_{-\infty}^{\mu} d\lambda \xi(\lambda, H_0, H(s))$ the integrated spectral shift function for the pair $(H_0, H(s))$, we prove concavity of $\zeta(\mu, s)$ with respect to s , extending previous results by Geisler, Kostykin, and Schrader. Our proofs employ operator-valued Herglotz functions and establish the latter as an effective tool in this context.

1. INTRODUCTION AND PRINCIPAL RESULTS

In the following \mathcal{H} denotes a complex separable Hilbert space with scalar product $(\cdot, \cdot)_{\mathcal{H}}$ (linear in the second factor) and norm $\|\cdot\|_{\mathcal{H}}$, $\mathcal{B}(\mathcal{H})$ represents the Banach space of bounded linear operators defined on \mathcal{H} , $\mathcal{B}_p(\mathcal{H})$, $p \geq 1$ the standard Schatten-von Neumann ideals of $\mathcal{B}(\mathcal{H})$ (cf., e.g., [18], [32]) and \mathbb{C}_+ (resp., \mathbb{C}_-) the open complex upper (resp., lower) half-plane. Moreover, real and imaginary parts of a bounded operator $T \in \mathcal{B}(\mathcal{H})$ are defined as usual by $\text{Re}(T) = (T + T^*)/2$, $\text{Im}(T) = (T - T^*)/(2i)$.

The spectral shift function $\xi(\lambda, H_0, H)$ associated with a pair of self-adjoint operators (H_0, H) , $H = H_0 + V$, $\text{dom}(H_0) = \text{dom}(H)$, where

$$V = V^* \in \mathcal{B}_1(\mathcal{H}), \quad (1.1)$$

is one of the fundamental spectral characteristics in the perturbation theory of self-adjoint operators. It is well-known (see [23], [24], [25], [26], [27]) that for a wide function class $\mathfrak{K}(H_0, H)$, the Lifshits-Krein trace formula holds, that is,

$$\text{tr}(\varphi(H) - \varphi(H_0)) = \int_{\mathbb{R}} d\lambda \varphi'(\lambda) \xi(\lambda, H_0, H), \quad \varphi \in \mathfrak{K}(H_0, H). \quad (1.2)$$

In the case of trace class perturbations (1.1), the spectral shift function is integrable, that is,

$$\xi(\cdot, H_0, H) \in L^1(\mathbb{R}), \quad (1.3)$$

and the following relations hold

$$\|\xi(\cdot, H_0, H)\|_{L^1(\mathbb{R})} \leq \|V\|_{\mathcal{B}_1(\mathcal{H})}, \quad (1.4)$$

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$$\int_{\mathbb{R}} d\lambda \, \xi(\lambda, H_0, H) = \operatorname{tr}(V). \quad (1.5)$$

The precise characterization of the class

$$\mathfrak{K} = \bigcap_{H_0, H} \mathfrak{K}(H_0, H) \quad (1.6)$$

of all those φ for which (1.2) holds for any pair of self-adjoint operators H_0 and $H = H_0 + V$ with a trace class difference (1.1), is still unknown. In particular, there are functions $\varphi \in C_0^1(\mathbb{R})$ for which (1.2) fails (cf. [11], [30]). Necessary conditions very close to sufficient ones for φ belonging to the class \mathfrak{K} have been found by Peller [28], [29]. Here we only note that (1.3) and $(\varphi(H) - \varphi(H_0)) \in \mathcal{B}_1(\mathcal{H})$ hold, and (1.2) is valid, if φ' is the Fourier transform of a finite Borel measure,

$$\varphi'(\lambda) = \int_{\mathbb{R}} d\nu(t) e^{-it\lambda}, \quad \varphi \in C^1(\mathbb{R}), \quad \int_{\mathbb{R}} d|\nu(t)| < \infty. \quad (1.7)$$

We denote the function class (1.7) by $\mathcal{W}_1(\mathbb{R})$.

Different representations for the spectral shift function and their interrelationships can be found in [4], for further information we refer to [2, Ch. 19], [9], [10], [16], [34, Ch. 8] and the references therein.

In the present short note we will focus on two particular results: one, a monotonicity result obtained by Birman and Solomyak [8], the other, a concavity result obtained by Geisler, Kostykin, and Schrader [12], [21]. We also present some extensions and new proofs that we hope might give additional insights into the subject.

We start by recalling pertinent results discovered by Birman and Solomyak [8] in connection with the spectral averaging formula (providing a representation for the spectral shift function via an integral over the coupling constant) and a monotonicity result of a certain trace with respect to the coupling constant parameter.

Theorem 1.1 ([8]). *Let H_0 and V be self-adjoint in \mathcal{H} , $V \in \mathcal{B}_1(\mathcal{H})$, and define*

$$H_s = H_0 + sV, \quad \operatorname{dom}(H_s) = \operatorname{dom}(H_0), \quad s \in \mathbb{R}, \quad (1.8)$$

with $\{E_{H_s}(\lambda)\}_{\lambda \in \mathbb{R}}$ the family of orthogonal spectral projections of H_s . Moreover, denote by $\xi(\cdot, H_0, H_1)$ the spectral shift function for the pair (H_0, H_1) . Then for any Borel set $\Delta \subset \mathbb{R}$,

$$\int_{\Delta} d\lambda \, \xi(\lambda, H_0, H_1) = \int_0^1 ds \operatorname{tr}(V E_{H_s}(\Delta)). \quad (1.9)$$

In the same paper [8], Birman and Solomyak proved another remarkable statement concerning the monotonicity of the integrand in the right-hand side of (1.9) with respect to s for semi-infinite intervals $\Delta = (-\infty, \lambda)$, $\lambda \in \mathbb{R}$.

Theorem 1.2 ([8]). *Assume the hypotheses in Theorem 1.1. Given $\mu \in \mathbb{R}$, the function*

$$s \longmapsto \operatorname{tr}(V E_{H_s}((-\infty, \mu))), \quad s \in \mathbb{R}, \quad (1.10)$$

is a nonincreasing function with respect to $s \in \mathbb{R}$.

The spectral averaging formula (1.9) combined with the monotonicity result (1.10) is a convenient tool for producing estimates for the spectral shift function

[8]. For instance,

$$\mathrm{tr} (VE_{H_1}((-\infty, \mu))) \leq \int_{-\infty}^{\mu} d\lambda \xi(\lambda, H_0, H_1) \leq \mathrm{tr} (VE_{H_0}((-\infty, \mu))). \quad (1.11)$$

In particular, passing to the limit $\mu \rightarrow \infty$ in (1.11) one obtains (1.5) (see [8] for more details).

Another application of the pair of results (1.9) and (1.10) leads to the proof of concavity properties of the integrated spectral shift function with respect to the coupling constant, originally discovered in the case of Schrödinger operators by Geisler, Kostykin, and Schrader [12] and extended by Kostykin [21], [22] to the general case presented next.

Theorem 1.3 ([21], [22]). *Let $\xi(\cdot, H_0, H_s)$ be the spectral shift function in Theorem 1.1. Given $\mu \in \mathbb{R}$, the integrated spectral shift function*

$$\zeta_s(\mu) = \int_{-\infty}^{\mu} d\lambda \xi(\lambda, H_0, H_s), \quad s \in \mathbb{R} \quad (1.12)$$

is a concave function with respect to the coupling constant $s \in \mathbb{R}$. More precisely, for any $s, t \in \mathbb{R}$, and for all $\alpha \in [0, 1]$, the following inequality

$$\zeta_{\alpha s + (1-\alpha)t}(\mu) \geq \alpha \zeta_s(\mu) + (1-\alpha) \zeta_t(\mu) \quad (1.13)$$

holds. Moreover, $\zeta_s(\mu)$ is subadditive with respect to $s \in (0, \infty)$ in the sense that for any $s, t \geq 0$,

$$\zeta_{s+t}(\mu) \leq \zeta_s(\mu) + \zeta_t(\mu). \quad (1.14)$$

While Theorem 1.3 focuses on a linear coupling constant dependence in $H_s = H_0 + sV$, Kostykin [21] also discusses the case of a nonlinear dependence on s for operators of the form $H(s) = H_0 + V(s)$:

Theorem 1.4 ([21], [22]). *Suppose $f : \mathbb{R} \rightarrow \mathbb{R}$ is an nonincreasing function of bounded variation and $\{V(s)\}_{s \in \mathbb{R}} \in \mathcal{B}_1(\mathcal{H})$ is operator concave (i.e., $V(\alpha s + (1-\alpha)t) \geq \alpha V(s) + (1-\alpha)V(t)$ for all $\alpha \in [0, 1]$, $s, t \in \mathbb{R}$). Then*

$$s \longmapsto g(V(s)) = \int_{\mathbb{R}} d\lambda f(\lambda) \xi(\lambda, H_0, H_0 + V(s)), \quad (1.15)$$

is concave in $s \in \mathbb{R}$. More precisely, for all $0 \leq \alpha \leq 1$ and all $s, t \in \mathbb{R}$, the following inequality

$$g(V(\alpha s + (1-\alpha)t)) \geq \alpha g(V(s)) + (1-\alpha)g(V(t)) \quad (1.16)$$

holds.

Actually, Kostykin considered the general case of relative trace class perturbations in [21] but we omit further details in this note.

Remark 1.5. The results of Theorems 1.1 and 1.2 in [8] have been obtained using the approach of Stieltjes' double operator integrals [5]–[7]. Birman and Solomyak treated the case $V(s) = sV$, $V \in \mathcal{B}_1(\mathcal{H})$, that is, they discussed the case of a linear dependence of the perturbation $V(s)$ with respect to the coupling constant parameter s . The general case of a nonlinear dependence $V(s)$ of s , assuming $V'(s) \geq 0$, in the context of the spectral averaging result (1.9) has recently been treated by Simon [33]. In Theorem 1.7 below we cite the most recent result of this type obtained in [16].

It is convenient to introduce the following hypothesis.

Hypothesis 1.6. *Let H_0 be a self-adjoint operator in \mathcal{H} with domain $\text{dom}(H_0)$, and assume $\{V(s)\}_{s \in \Omega} \subset \mathcal{B}_1(\mathcal{H})$ to be a family of self-adjoint trace class operators in \mathcal{H} , where $\Omega \subseteq \mathbb{R}$ denotes an open interval with $0 \in \Omega$. Moreover, suppose that $V(s)$ is continuously differentiable in $\mathcal{B}_1(\mathcal{H})$ -norm with respect to $s \in \Omega$. For convenience (and without loss of generality) we may assume that $V(0) = 0$ in the following.*

In the rest of the paper we will frequently use the notation $(s_1, s_2) \subset\subset \Omega$ to denote an open interval that is strictly contained in the interval $\Omega = (a, b)$ (i.e., $a < s_1 < s_2 < b$).

Theorem 1.7 ([16]). *Assume Hypothesis 1.6 and $0 \in (s_1, s_2) \subset\subset \Omega$. Let*

$$H(s) = H_0 + V(s), \quad \text{dom}(H(s)) = \text{dom}(H_0), \quad s \in (s_1, s_2), \quad (1.17)$$

with $\{E_{H(s)}(\lambda)\}_{\lambda \in \mathbb{R}}$ the family of orthogonal spectral projections of $H(s)$ and denote by $\xi(\cdot, H_0, H(s))$ the spectral shift function for the pair $(H_0, H(s))$. Then for any Borel set $\Delta \subset \mathbb{R}$ the following spectral averaging formula holds

$$\int_{\Delta} d\lambda (\xi(\lambda, H_0, H(s_2)) - \xi(\lambda, H_0, H(s_1))) = \int_{s_1}^{s_2} ds \, \text{tr}(V'(s)E_{H(s)}(\Delta)). \quad (1.18)$$

The principal new result of the present note is an extension of the monotonicity result, Theorem 1.2, to the case of a nonlinear dependence of $V(s)$ on s . In particular, we provide a new strategy of proof for such results, which appears to be interesting in itself.

Theorem 1.8. *Assume Hypothesis 1.6 and $0 \in (s_1, s_2) \subset\subset \Omega$. Suppose in addition, that the derivative $V'(s)$ is continuously differentiable in $\mathcal{B}_1(\mathcal{H})$ -norm with respect to $s \in (s_1, s_2)$ and that $V(s)$ is concave in the sense that*

$$0 \geq V''(s) \in \mathcal{B}_1(\mathcal{H}), \quad s \in (s_1, s_2). \quad (1.19)$$

Then, given $\mu \in \mathbb{R}$, the function

$$s \longmapsto \text{tr}(V'(s)E_{H(s)}((-\infty, \mu))), \quad s \in (s_1, s_2), \quad (1.20)$$

is a nonincreasing function with respect to $s \in (s_1, s_2)$.

Combining Theorems 1.7 and 1.8 one obtains the following result.

Corollary 1.9. *Suppose the hypotheses of Theorem 1.8. Then, for given $\mu \in \mathbb{R}$, the integrated spectral shift function*

$$\zeta(\mu, s) = \int_{-\infty}^{\mu} d\lambda \xi(\lambda, H_0, H(s)) \quad (1.21)$$

is concave in $s \in (s_1, s_2)$. More precisely, for all $0 \leq \alpha \leq 1$ and all $s, t \in (s_1, s_2)$, the following inequality

$$\zeta(\mu, \alpha s + (1 - \alpha)t) \geq \alpha \zeta(\mu, s) + (1 - \alpha) \zeta(\mu, t) \quad (1.22)$$

holds. Moreover, $\zeta(\mu, s)$ is subadditive with respect to $s \in [0, s_2)$ in the sense that for any $s, t \geq 0$, $s + t \in [0, s_2)$,

$$\zeta(\mu, s + t) \leq \zeta(\mu, s) + \zeta(\mu, t). \quad (1.23)$$

We emphasize that Corollary 1.9 is a special case of Kostykin's Theorem 1.4.

As explained in [3], [8], and [9], the original proofs of Theorems 1.1 and 1.2 in [8] were motivated by a real analysis approach to the spectral shift function in contrast to M. Krein's complex analytic treatment. In this note we return to complex analytic proofs in the spirit of M. Krein and provide a proof of the monotonicity result, Theorem 1.8, based on operator-valued Herglotz function techniques. For various recent applications of this formalism we refer to [13], [14], [15], [16], and [17].

2. A PROPERTY OF OPERATOR-VALUED HERGLOTZ FUNCTIONS

We recall that $f : \mathbb{C}_+ \rightarrow \mathbb{C}$ is called a *Herglotz function* if it is analytic and $f(\mathbb{C}_+) \subseteq \overline{\mathbb{C}_+}$. In this case we extend f to \mathbb{C}_- in the usual manner, that is, by $f(\bar{z}) = \overline{f(z)}$, $z \in \mathbb{C}_+$.

The principal purpose of this section is to obtain some generalizations of the following elementary result.

Lemma 2.1. *Let P and Q be two rational Herglotz functions vanishing at infinity and let Γ be a closed clockwise oriented Jordan contour encircling some of the poles of P and Q starting from the left (and without any poles of P and Q on Γ). Then*

$$\frac{1}{2\pi i} \oint_{\Gamma} dz P(z)Q(z) \geq 0. \quad (2.1)$$

Proof. By the hypotheses on P and Q we may write

$$P(z) = \sum_{j \in J_1} A_j (p_j - z)^{-1}, \quad A_j \geq 0, \quad p_j \in \mathbb{R}, \quad j \in J_1, \quad (2.2)$$

$$Q(z) = \sum_{\ell \in J_2} B_{\ell} (q_{\ell} - z)^{-1}, \quad B_{\ell} \geq 0, \quad q_{\ell} \in \mathbb{R}, \quad \ell \in J_2, \quad (2.3)$$

$$(2.4)$$

with J_1, J_2 finite index sets. Next one decomposes P and Q with respect to their poles located in the interior and exterior of the bounded domain encircled by Γ ,

$$\begin{aligned} P(z) &= P_{\text{int}}(z) + P_{\text{ext}}(z) \\ &= \sum_{j \in J_{1,\text{int}}} A_j (p_j - z)^{-1} + \sum_{j \in J_{1,\text{ext}}} A_j (p_j - z)^{-1}, \end{aligned} \quad (2.5)$$

$$\begin{aligned} Q(z) &= Q_{\text{int}}(z) + Q_{\text{ext}}(z) \\ &= \sum_{\ell \in J_{2,\text{int}}} B_{\ell} (q_{\ell} - z)^{-1} + \sum_{\ell \in J_{2,\text{ext}}} B_{\ell} (q_{\ell} - z)^{-1}, \end{aligned} \quad (2.6)$$

$$J_k = J_{k,\text{int}} \cup J_{k,\text{ext}}, \quad k = 1, 2. \quad (2.7)$$

Then straightforward residue computations yield

$$\begin{aligned} &\frac{1}{2\pi i} \oint_{\Gamma} dz P(z)Q(z) \\ &= \frac{1}{2\pi i} \oint_{\Gamma} dz P_{\text{int}}(z)Q_{\text{int}}(z) + \frac{1}{2\pi i} \oint_{\Gamma} dz P_{\text{int}}(z)Q_{\text{ext}}(z) \\ &\quad + \frac{1}{2\pi i} \oint_{\Gamma} dz P_{\text{ext}}(z)Q_{\text{int}}(z) + \frac{1}{2\pi i} \oint_{\Gamma} dz P_{\text{ext}}(z)Q_{\text{ext}}(z) \end{aligned} \quad (2.8)$$

$$\begin{aligned}
&= \frac{1}{2\pi i} \oint_{\Gamma} dz \sum_{j \in J_{1,\text{int}}} \sum_{\ell \in J_{2,\text{int}}} A_j B_{\ell} (p_j - z)^{-1} (q_{\ell} - z)^{-1} \\
&\quad + \sum_{j \in J_{1,\text{int}}} A_j Q_{\text{ext}}(p_j) + \sum_{\ell \in J_{2,\text{int}}} B_{\ell} P_{\text{ext}}(q_{\ell}) \\
&= \frac{1}{2\pi i} \oint_{\Gamma} dz \sum'_{j \in J_{1,\text{int}}, \ell \in J_{2,\text{int}}} A_j B_{\ell} (q_{\ell} - p_j)^{-1} ((q_{\ell} - z)^{-1} - (p_j - z)^{-1}) \\
&\quad + \sum_{j \in J_{1,\text{int}}} A_j Q_{\text{ext}}(p_j) + \sum_{\ell \in J_{2,\text{int}}} B_{\ell} P_{\text{ext}}(q_{\ell}) \tag{2.9}
\end{aligned}$$

$$\begin{aligned}
&= \sum_{j \in J_{1,\text{int}}} A_j Q_{\text{ext}}(p_j) + \sum_{\ell \in J_{2,\text{int}}} B_{\ell} P_{\text{ext}}(q_{\ell}) \\
&= \sum_{j \in J_{1,\text{int}}} \sum_{\ell \in J_{2,\text{ext}}} A_j B_{\ell} (q_{\ell} - p_j)^{-1} + \sum_{j \in J_{1,\text{ext}}} \sum_{\ell \in J_{2,\text{int}}} A_j B_{\ell} (p_j - q_{\ell})^{-1} \geq 0. \tag{2.10}
\end{aligned}$$

Here the last integral in (2.8) vanishes since the integrand is analytic inside Γ and the first integral in (2.9) vanishes by symmetry. Moreover, we used the symbol \sum' to indicate summation only over those j and ℓ with $p_j \neq q_{\ell}$, since only first-order poles contribute in this calculation. \square

Next we turn to operator-valued extensions of the concept of Herglotz functions.

Definition 2.2. $M : \mathbb{C}_+ \rightarrow \mathcal{B}(\mathcal{H})$ is called an *operator-valued Herglotz function* if M is analytic on \mathbb{C}_+ and $\text{Im}(M(z)) \geq 0$ for all $z \in \mathbb{C}_+$.

Any operator-valued Herglotz function admits a canonical representation, which can be considered a generalization of the dilation theory of maximal dissipative operators to the case of operator-valued Herglotz functions. In the following, however, we will focus on Herglotz functions of the resolvent-type

$$M(z) = K^*(L - z)^{-1}K, \quad z \in \mathbb{C}_+, \tag{2.11}$$

where K is a bounded operator between the Hilbert spaces \mathcal{K} and \mathcal{H} , $K \in \mathcal{B}(\mathcal{H}, \mathcal{K})$, $\mathcal{K} \supseteq \mathcal{H}$, while L is assumed to be a self-adjoint operator in \mathcal{K} , bounded from below, and with a gap in its spectrum as described in Theorem 2.3 below.

Theorem 2.3. Let $M_j : \mathbb{C}_+ \rightarrow \mathcal{B}_2(\mathcal{H})$, $j = 1, 2$, be operator-valued Herglotz functions (taking values in the space of the Hilbert-Schmidt operators) admitting the representations

$$M_j(z) = K_j(L_j - z)^{-1}K_j^*, \tag{2.12}$$

where \mathcal{K}_j and \mathcal{H} , $\mathcal{K}_j \supseteq \mathcal{H}$, are Hilbert spaces, L_j are self-adjoint operators in \mathcal{K}_j bounded from below, and $K_j \in \mathcal{B}_4(\mathcal{K}_j, \mathcal{H})$, $j = 1, 2$. Suppose \mathcal{D} is a domain in the complex plane and (a, b) an open interval such that

$$a < \min_{j=1,2} \inf(\text{spec}(L_j)) \tag{2.13}$$

and

$$\{\text{spec}(L_1) \cup \text{spec}(L_2)\} \cap \mathcal{D} \subset (a, b) \subset \mathcal{D}. \tag{2.14}$$

In addition, assume that Γ is a closed oriented Jordan contour in \mathcal{D} encircling the interval $[a, b]$ in the clockwise direction, and φ an analytic function on \mathcal{D} , nonnegative and nonincreasing on (a, b) , that is,

$$\varphi|_{(a,b)} \geq 0, \quad (2.15)$$

and

$$\varphi'|_{(a,b)} \leq 0. \quad (2.16)$$

Then

$$\frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (M_1(z) M_2(z)) \geq 0. \quad (2.17)$$

Proof. Given $n \in \mathbb{N}$, introduce the partition $a = t_0 < t_1 < t_2 < \dots < t_{n-1} < t_n = b$ of the closed interval $[a, b]$,

$$t_k = a + k \frac{b-a}{n}, \quad k = 1, 2, \dots, n, \quad (2.18)$$

and denote by $\chi^{(n)}(\lambda)$ the piecewise continuous function

$$\chi^{(n)}(\lambda) = \sum_{k=1}^n t_k \chi_{[t_{k-1}, t_k)}(\lambda), \quad \lambda \in \mathbb{R}, \quad (2.19)$$

where $\chi_{\Delta}(\cdot)$ is the characteristic function of the set $\Delta \subset \mathbb{R}$.

In the Hilbert space \mathcal{K}_j introduce the (possibly unbounded) operators

$$L_j^{(n)} = \int_{(a,b)} \chi^{(n)}(\lambda) dE_{L_j}(\lambda) + \int_{(b,\infty)} \lambda dE_{L_j}(\lambda), \quad (2.20)$$

$$\operatorname{dom}(L_j^{(n)}) = \operatorname{dom}(L_j), \quad n \in \mathbb{N}, \quad j = 1, 2.$$

We note, that by definition (2.20), the spectrum of L_j , $j = 1, 2$, in the interval (a, b) consists of finitely many eigenvalues (possibly of infinite multiplicity).

By (2.14) one infers that the sequence of operators $\{L_j^{(n)}\}_{n=1}^{\infty}$ converges in norm resolvent sense to L_j in the Hilbert space \mathcal{K}_j , $j = 1, 2$. This convergence, in turn, combined with the hypothesis $K_j \in \mathcal{B}_4(\mathcal{K}_j, \mathcal{H})$, $j = 1, 2$, implies the convergence

$$\lim_{n \rightarrow \infty} \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (M_1^{(n)}(z) M_2^{(n)}(z)) = \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (M_1(z) M_2(z)), \quad (2.21)$$

where in obvious notation

$$M_j^{(n)}(z) = K_j (L_j^{(n)} - z)^{-1} K_j^*, \quad j = 1, 2. \quad (2.22)$$

Thus, in order to prove (2.17) it suffices to check that every term on the left-hand side of (2.21) is nonnegative.

In the following it is useful to decompose the Herglotz functions $M_j^{(n)}(z)$ in the form

$$M_j^{(n)}(z) = N_j^{(n)}(z) + \tilde{N}_j^{(n)}(z), \quad j = 1, 2, \quad (2.23)$$

where

$$N_j^{(n)}(z) = K_j E_{L_j}((a, b)) (L_j^{(n)} - z)^{-1} E_{L_j}((a, b)) K_j^*, \quad (2.24)$$

$$\tilde{N}_j^{(n)}(z) = K_j E_{L_j}([b, \infty)) (L_j^{(n)} - z)^{-1} E_{L_j}([b, \infty)) K_j^*, \quad j = 1, 2 \quad (2.25)$$

are Herglotz functions associated with the spectral subspaces $E_{L_j}((a, b))\mathcal{K}_j$ and $E_{L_j}([b, \infty))\mathcal{K}_j$ of L_j , $j = 1, 2$.

According to the decomposition (2.20), the Herglotz functions $N_j^{(n)}(z)$ are rational operator-valued functions of the form

$$N_j^{(n)}(z) = \sum_{k=1}^n \frac{Q_j^{(n),k}}{t_k - z}, \quad j = 1, 2, \quad (2.26)$$

where

$$Q_j^{(n),k} = K_j E_{L_j}([t_{k-1}, t_k)) K_j^* \geq 0, \quad k = 1, \dots, n, \quad j = 1, 2. \quad (2.27)$$

Given $n \in \mathbb{N}$, one decomposes the integrals on the left-hand side of (2.21) as a sum of four terms

$$\begin{aligned} \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (M_1^{(n)}(z) M_2^{(n)}(z)) &= \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (N_1^{(n)}(z) N_2^{(n)}(z)) \\ &\quad + \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (\tilde{N}_1^{(n)}(z) \tilde{N}_2^{(n)}(z)) \\ &\quad + \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (\tilde{N}_1^{(n)}(z) N_2^{(n)}(z)) \\ &\quad + \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr} (N_1^{(n)}(z) \tilde{N}_2^{(n)}(z)) \\ &= J_1 + J_2 + J_3 + J_4. \end{aligned} \quad (2.28)$$

According to (2.26), the first integral J_1 in (2.28) can be represented as follows

$$\begin{aligned} J_1 &= \frac{1}{2\pi i} \sum_{k,m}^n \oint_{\Gamma} dz \frac{\varphi(z)}{(t_k - z)(t_m - z)} \operatorname{tr}(Q_1^{(n),k} Q_2^{(n),m}) \\ &= \frac{1}{2\pi i} \sum_{\substack{k,m \\ k \neq m}}^n \oint_{\Gamma} dz \frac{\varphi(z)}{(t_k - z)(t_m - z)} \operatorname{tr}(Q_1^{(n),k} Q_2^{(n),m}) \\ &\quad + \frac{1}{2\pi i} \sum_{k=1}^n \oint_{\Gamma} dz \frac{\varphi(z)}{(t_k - z)^2} \operatorname{tr}(Q_1^{(n),k} Q_2^{(n),k}). \end{aligned} \quad (2.29)$$

Applying the residue theorem to the integrals on the right-hand side of (2.29) one infers

$$\begin{aligned} J_1 &= \sum_{\substack{k,m \\ k \neq m}}^n \left(-\frac{\varphi(t_k) - \varphi(t_m)}{t_k - t_m} \right) \operatorname{tr}(Q_1^{(n),k} Q_2^{(n),m}) \\ &\quad - \sum_{k=1}^n \varphi'(t_k) \operatorname{tr}(Q_1^{(n),k} Q_2^{(n),k}) \geq 0, \end{aligned} \quad (2.30)$$

since φ is a nonincreasing differentiable function and since the inequalities

$$\operatorname{tr}(Q_1^{(n),k} Q_2^{(n),m}) \geq 0, \quad k, m = 1, \dots, n \quad (2.31)$$

hold (due to the fact that the operators $Q_j^{(n),k}$, $k = 1, 2, \dots, n$, $j = 1, 2$, are nonnegative by (2.27)).

The integral J_2 vanishes,

$$J_2 = 0, \quad (2.32)$$

since $\text{tr}(\tilde{N}_1^{(n)}(z)\tilde{N}_2^{(n)}(z))$ is holomorphic in \mathcal{D} .

The remaining integrals J_3 and J_4 can also be evaluated by the residue theorem and one obtains

$$J_3 = \sum_{k=1}^n \varphi(t_k) \text{tr}(\tilde{N}_1^{(n)}(t_k)Q_2^{(n),k}), \quad (2.33)$$

$$J_4 = \sum_{k=1}^n \varphi(t_k) \text{tr}(Q_1^{(n),k}\tilde{N}_2^{(n)}(t_k)). \quad (2.34)$$

We recall that $\varphi(t_k) \geq 0$, $k = 1, \dots, n$, by (2.15). At the same time

$$\tilde{N}_j^{(n)}(t_k) \geq 0, \quad k = 1, 2, \dots, n, \quad n \in \mathbb{N}, \quad j = 1, 2, \quad (2.35)$$

by (2.20) and (2.25), while

$$Q_j^{(n),k} \geq 0, \quad k = 1, 2, \dots, n, \quad n \in \mathbb{N}, \quad j = 1, 2, \quad (2.36)$$

by (2.27). Hence,

$$\text{tr}(\tilde{N}_1^{(n)}(t_k)Q_2^{(n),k}) \geq 0 \text{ and } \text{tr}(Q_1^{(n),k}\tilde{N}_2^{(n)}(t_k)) \geq 0, \quad k = 1, \dots, n, \quad (2.37)$$

and thus, $J_3 \geq 0$ and $J_4 \geq 0$. Together with (2.30) and (2.32) (combined with (2.21)) this proves (2.17). \square

Remark 2.4. (i) Conditions $K_j \in \mathcal{B}_4(\mathcal{K}_j, \mathcal{H})$, $j = 1, 2$, in Theorem 2.3 can be relaxed. In fact, it suffices to require that

$$M_1(z)M_2(z) \in \mathcal{B}_1(\mathcal{H}), \quad z \in \mathbb{C}_+. \quad (2.38)$$

(ii) Hypotheses (2.13) and (2.14) concerning the semiboundedness of L_j , $j = 1, 2$, and the existence of a gap in their spectra in Theorem 2.3, are also unnecessarily stringent. In fact, it suffices to assume that the holomorphy domains of the Herglotz functions $M_j(z)$ $j = 1, 2$ given by (2.12) include the set $(-\infty, \alpha) \cup (\beta, \gamma)$ for some $a < \alpha$ and $b < \beta < \gamma$.

(iii) If the operators L_j are bounded and

$$\text{spec}(L_j) \subset (a, b), \quad j = 1, 2, \quad (2.39)$$

then the terms (2.25) in the decomposition (2.23) vanish and hence the integrals (2.33) and (2.34) vanish too. This means that under assumption (2.39), condition (2.15) is redundant.

3. MONOTONICITY, CONCAVITY, AND SUBADDITIVITY

Throughout this section we assume Hypothesis 1.6 and recall that

$$H(s) = H_0 + V(s), \quad \text{dom}(H(s)) = \text{dom}(H_0), \quad s \in \Omega. \quad (3.1)$$

First, we treat the case of bounded H_0 , $H_0 \in \mathcal{B}(\mathcal{H})$, and study differential and monotonicity properties of the function

$$s \longmapsto \text{tr}(V'(s)\varphi(H(s))), \quad s \in \Omega, \quad (3.2)$$

where φ is analytic on a domain \mathcal{D} containing the spectra of the family (3.1)

$$\bigcup_{s \in \Omega} (\text{spec}(H(s))) \subset \mathcal{D}. \quad (3.3)$$

Next we introduce the following additional hypothesis, which is motivated in part by Remark 2.4 (iii).

Hypothesis 3.1. *Let H be a bounded self-adjoint operator, \mathcal{D} a domain of the complex plane, $(a, b) \subset \mathbb{R}$ an open interval, and Γ a closed clockwise oriented Jordan contour in \mathcal{D} encircling the interval $[a, b]$ such that*

$$\text{spec}(H) \subset (a, b) \subset \mathcal{D}. \quad (3.4)$$

The following remark shows that Hypothesis 3.1 is stable under small (compact) perturbations of H .

Remark 3.2. Suppose that the collection $\{H(s_0), \mathcal{D}, (a, b), \Gamma\}$ satisfies Hypothesis 3.1 for some $s_0 \in (s_1, s_2)$. By perturbation arguments, one infers the existence of a neighborhood S of s_0 such that $\{H(s), \mathcal{D}, (a, b), \Gamma\}$ also satisfy Hypothesis 3.1 for $s \in S$. Moreover, if φ is analytic on \mathcal{D} , then the (bounded) operators $\varphi(H(s))$, $s \in S$, are well-defined by the Riesz integral

$$\varphi(H(s)) = \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) (H(s) - z)^{-1}, \quad s \in S. \quad (3.5)$$

Lemma 3.3. *Assume Hypothesis 1.6 and let S be the neighborhood of s_0 in Remark 3.2. Suppose in addition that $V'(s)$ is continuously differentiable in $\mathcal{B}_1(\mathcal{H})$ -norm for $s \in S$ and that the collection $\{H(s_0), \mathcal{D}, (a, b), \Gamma\}$ satisfies Hypothesis 3.1 for some $s_0 \in (s_1, s_2)$. If φ is an analytic function on \mathcal{D} , then*

$$s \mapsto \text{tr}(V'(s) \varphi(H(s))), \quad s \in S, \quad (3.6)$$

is differentiable on S and

$$\begin{aligned} \frac{d}{ds} \text{tr}(V'(s) \varphi(H(s))) &= \text{tr}(V''(s) \varphi(H(s))) \\ &\quad - \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \text{tr}[V'(s)(H(s) - z)^{-1}]^2. \end{aligned} \quad (3.7)$$

Proof. By Remark 3.2, the operators $\varphi(H(s))$, $s \in S$, are well-defined (cf. (3.5)). In particular,

$$\begin{aligned} \frac{\varphi(H(s)) - \varphi(H(s_0))}{s - s_0} &= \frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \frac{(H(s) - z)^{-1} - (H(s_0) - z)^{-1}}{s - s_0} \\ &= -\frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) (H(s) - z)^{-1} \frac{V(s) - V(s_0)}{s - s_0} (H(s_0) - z)^{-1}. \end{aligned} \quad (3.8)$$

Since $n\text{-}\lim_{s \rightarrow s_0} H(s) = H(s_0)$, one infers

$$n\text{-}\lim_{s \rightarrow s_0} (H(s) - z)^{-1} = (H(s_0) - z)^{-1}, \quad (3.9)$$

uniformly with respect to $z \in \Gamma$. Thus, combining (3.9) and (3.8), one concludes that $s \mapsto \varphi(H(s))$ is differentiable with respect to $s \in S$ in $\mathcal{B}(\mathcal{H})$ -topology. Along with the existence of a continuous $V''(s)$ on S , this yields the differentiability of the function in (3.6). Equation (3.7) then follows by a straightforward computation using (3.5). \square

Lemma 3.4. *Under the assumptions of Lemma 3.3 suppose in addition that $V(s)$ is concave with respect to $s \in S$ in the sense that*

$$0 \geq V''(s) \in \mathcal{B}_1(\mathcal{H}), \quad s \in S, \quad (3.10)$$

and that the function φ is nonnegative and nonincreasing on (a, b) . Then the function

$$s \mapsto \operatorname{tr}(V'(s) \varphi(H(s))), \quad s \in S, \quad (3.11)$$

is differentiable and nonincreasing on S .

Proof. Since φ is nonnegative, $0 \leq \varphi(H(s)) \in \mathcal{B}(\mathcal{H})$, $s \in S$ and hence

$$\operatorname{tr}(V''(s) \varphi(H(s))) \leq 0, \quad s \in S, \quad (3.12)$$

by (3.10). Applying Theorem 2.3 and Remark 2.4 (i) to the operator-valued Herglotz functions $M_1(z) = V'(s)(H(s) - z)^{-1}V'(s)$ and $M_2(z) = (H(s) - z)^{-1}$, one obtains the inequality

$$\frac{1}{2\pi i} \oint_{\Gamma} dz \varphi(z) \operatorname{tr}[V'(s)(H(s) - z)^{-1}]^2 \geq 0, \quad s \in S. \quad (3.13)$$

Combining (3.12) and (3.13) one infers

$$\frac{d}{ds} \operatorname{tr}(V'(s) \varphi(H(s))) \leq 0 \quad (3.14)$$

by Lemma 3.3, proving the assertion. \square

In the general case of unbounded operators H_0 one can prove the following result.

Theorem 3.5. *Assume Hypothesis 1.6. Suppose in addition that $V'(s)$ is continuously differentiable in $\mathcal{B}_1(\mathcal{H})$ -norm with respect to $s \in (s_1, s_2)$ and that $V(s)$ is concave in the sense that*

$$0 \geq V''(s) \in \mathcal{B}_1(\mathcal{H}), \quad s \in (s_1, s_2). \quad (3.15)$$

Let φ be a bounded nonnegative and nonincreasing real-analytic function on \mathbb{R} admitting the analytic continuation to a domain \mathcal{D} of the complex plane \mathbb{C} containing the real axis \mathbb{R} . Then the function

$$s \mapsto \operatorname{tr}(V'(s) \varphi(H(s))), \quad s \in (s_1, s_2), \quad (3.16)$$

is nonincreasing with respect to $s \in (s_1, s_2)$.

Proof. Introducing the sequence $\{P_n\}_{n \in \mathbb{N}}$ of spectral projections of H_0 ,

$$P_n = E_{H_0}((-n, n)), \quad n \in \mathbb{N}, \quad (3.17)$$

one concludes that for fixed $s \in \mathbb{R}$ the bounded operators given by

$$H^{(n)}(s) = P_n H_0 P_n + V(s), \quad \operatorname{dom}(H^{(n)}(s)) = \mathcal{H}, \quad (3.18)$$

converge to $H(s)$ in the strong resolvent sense and therefore,

$$s\text{-}\lim_{n \rightarrow \infty} \varphi(H^{(n)}(s)) = \varphi(H(s)), \quad s \in (s_1, s_2), \quad (3.19)$$

by Theorem VIII.20 in [31].

Since by hypothesis φ is a bounded function, the family of operators $\varphi(H^{(n)}(s))$ is uniformly bounded with respect to n and hence by Theorem 1 in [19],

$$\lim_{n \rightarrow \infty} \operatorname{tr}(V'(s) \varphi(H^{(n)}(s))) = \operatorname{tr}(V'(s) \varphi(H(s))), \quad s \in (s_1, s_2). \quad (3.20)$$

Given $n \in \mathbb{N}$ and $s_0 \in (s_1, s_2)$, one can always find a closed oriented Jordan contour Γ in \mathcal{D} , and a bounded interval $(a, b) \subset \mathbb{R}$ such that the collection $\{H^{(n)}(s_0), \mathcal{D}, (a, b), \Gamma\}$ satisfies Hypothesis 3.1. Since by hypothesis φ is a nonnegative nonincreasing function on (a, b) and (3.15) holds, one concludes by Lemma 3.4 that the function

$$s \longmapsto \operatorname{tr}(V'(s) \varphi(H^{(n)}(s))) \quad (3.21)$$

is nonincreasing in some neighborhood of s_0 and hence on the whole interval (s_1, s_2) since $s_0 \in (s_1, s_2)$ was arbitrary. Therefore, the function

$$s \longmapsto \operatorname{tr}(V'(s) \varphi(H(s))), \quad s \in (s_1, s_2), \quad (3.22)$$

is also nonincreasing on (s_1, s_2) as a pointwise limit (3.20) of the nonincreasing functions in (3.21). \square

Now we are able to prove Theorem 1.8, which is an extension of the monotonicity result, Theorem 1.2, of Birman and Solomyak [8].

Proof of Theorem 1.8. Given $\mu \in \mathbb{R}$, introducing the real-analytic function

$$\varphi_{\mu, \varepsilon}(\lambda) = \frac{1}{2} - \frac{1}{\pi} \arctan \left(\frac{\lambda - \mu}{\varepsilon} + \frac{1}{\sqrt{\varepsilon}} \right), \quad \varepsilon > 0, \quad (3.23)$$

one concludes that

$$\lim_{\varepsilon \downarrow 0} \varphi_{\mu, \varepsilon}(\lambda) = \chi_{(-\infty, \mu)}(\lambda), \quad (3.24)$$

where $\chi_{\Delta}(\cdot)$ denotes the characteristic function of the set Δ .

Since

$$\sup_{\varepsilon > 0} \|\varphi_{\mu, \varepsilon}\|_{L^\infty(\mathbb{R})} < \infty, \quad (3.25)$$

(3.24) implies the strong convergence

$$s\text{-}\lim_{\varepsilon \downarrow 0} \varphi_{\mu, \varepsilon}(H(s)) = E_{H(s)}((-\infty, \mu)) \quad (3.26)$$

by Theorem VIII.5 in [31]. Combining (3.24)–(3.26) with Theorem 1 in [19], one infers

$$\lim_{\varepsilon \downarrow 0} \operatorname{tr}(V'(s) \varphi_{\mu, \varepsilon}(H(s))) = \operatorname{tr}(V'(s) E_{H(s)}((-\infty, \mu))). \quad (3.27)$$

By Theorem 1.8, the function

$$s \longmapsto \operatorname{tr}(V'(s) \varphi_{\mu, \varepsilon}(H(s))), \quad s \in (s_1, s_2), \quad (3.28)$$

is nonincreasing, proving the assertion, since the pointwise limit of nonincreasing functions is nonincreasing. \square

Next we prove Corollary 1.9.

Proof of Corollary 1.9. By Theorem 1.7

$$\int_{-\infty}^{\mu} d\lambda \xi(\lambda, H_0, H(s)) = \int_0^s dt \operatorname{tr}(V'(t) E_{H(t)}((-\infty, \mu))), \quad s \in (s_1, s_2), \quad \mu \in \mathbb{R}. \quad (3.29)$$

By Theorem 1.8 the integrand on the right-hand side of (3.29) is a nonincreasing function of t and hence the left-hand side of (3.29) is a concave function of s . Thus (1.22) holds.

In order to prove (1.23) one notes that $\zeta(\mu, 0+) = 0$ and that a necessary and sufficient condition for a measurable concave function $f(t)$ to be subadditive on $(0, \infty)$ is that $f(0+) \geq 0$ (see, e.g., [20, Theorem 7.2.5]). \square

In the case of semibounded operators the following statement might be useful. We recall that $\mathcal{W}_1(\mathbb{R})$ denotes the function class of φ with φ' the Fourier transform of a finite (complex) Borel measure (cf. (1.7)).

Theorem 3.6. *Let H_0 be a self-adjoint operator in \mathcal{H} , bounded from below, and assume the hypotheses of Theorem 1.8. Denote by Λ the smallest semi-infinite interval containing the spectra of the family $H(s)$, $s \in (s_1, s_2)$,*

$$\Lambda = \left[\inf_{s \in (s_1, s_2)} \text{spec}(H(s)), \infty \right). \quad (3.30)$$

Let $\varphi \in \mathcal{W}_1(\mathbb{R}) \cap C^2(\mathbb{R})$ be concave on Λ in the sense that

$$\varphi''|_{\Lambda} \leq 0, \quad (3.31)$$

and

$$\varphi'(\lambda) = o(1) \text{ as } \lambda \rightarrow +\infty. \quad (3.32)$$

Then the function

$$s \mapsto \text{tr}[\varphi(H(s)) - \varphi(H_0)], \quad s \in (s_1, s_2), \quad (3.33)$$

is concave in the sense that for any $s, t \in (s_1, s_2)$ and for any $0 \leq \alpha \leq 1$,

$$\begin{aligned} & \text{tr}[\varphi(H(\alpha s + (1 - \alpha)t)) - \varphi(H_0)] \\ & \geq \alpha \text{tr}[\varphi(H(s)) - \varphi(H_0)] + (1 - \alpha) \text{tr}[\varphi(H(t)) - \varphi(H_0)]. \end{aligned} \quad (3.34)$$

In particular,

$$[\varphi(H(\alpha s + (1 - \alpha)t)) - \alpha \varphi(H(s)) - (1 - \alpha) \varphi(H(t))] \in \mathcal{B}_1(\mathcal{H}) \quad (3.35)$$

and

$$\text{tr}[\varphi(H(\alpha s + (1 - \alpha)t)) - \alpha \varphi(H(s)) - (1 - \alpha) \varphi(H(t))] \geq 0. \quad (3.36)$$

Proof. First, one observes that by (1.4) the integrated spectral shift function $\zeta(\lambda, s)$ given by (1.21) is uniformly bounded, that is,

$$|\zeta(\lambda, s)| \leq \|V(s)\|_{\mathcal{B}_1(\mathcal{H})}, \quad \lambda \in \mathbb{R}, \quad s \in (s_1, s_2). \quad (3.37)$$

Moreover, since H_0 is semibounded, one concludes that $\mathbb{R} \setminus \Lambda \neq \emptyset$ by definition (3.30) of the set Λ and hence for all $s \in (s_1, s_2)$,

$$\zeta(\lambda, s) = 0, \quad \lambda \in \mathbb{R} \setminus \Lambda. \quad (3.38)$$

Thus, using (3.32) and (3.38), one infers

$$\lim_{\lambda \rightarrow \pm\infty} \varphi'(\lambda) \zeta(\lambda, s) = 0, \quad s \in (s_1, s_2). \quad (3.39)$$

Next, combining (3.38) and (3.39), an integration by parts in the trace formula (1.2) yields

$$\text{tr}[\varphi(H(s)) - \varphi(H_0)] = - \int_{\Lambda} d\lambda \varphi''(\lambda) \zeta(\lambda, s). \quad (3.40)$$

Given $\lambda \in \mathbb{R}$, the integrated spectral shift function $\zeta(\lambda, s)$ is concave with respect to $s \in (s_1, s_2)$ by Corollary 1.9 and hence the left-hand side of (3.40) is also a concave function of s by (3.31) (as a weighted mean of concave functions with a positive weight). \square

Remark 3.7. (i) If the measure ν in representation (1.7) is absolutely continuous, then condition (3.32) holds automatically by the Riemann–Lebesgue Lemma.

(ii) If φ is convex on Λ , that is,

$$\varphi''|_{\Lambda} \geq 0, \quad (3.41)$$

then the function given by (3.33) is convex.

Example 3.8. Under assumptions of Theorem 3.6, choosing $\varphi \in \mathcal{W}_1(\mathbb{R})$ as

$$\varphi(\lambda) = \exp(-\lambda t), \quad \lambda \in \Lambda, \quad t \geq 0, \quad (3.42)$$

one concludes that for any $t > 0$,

$$s \longrightarrow \operatorname{tr}[\exp(-tH(s)) - \exp(-tH_0)] \quad (3.43)$$

is a convex function of $s \in (s_1, s_2)$.

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